

Aim

To understand the effect of Bose-Einstein statistics on the thermodynamic properties of bosons.

Objectives

- 1. To derive the heat capacity of a solid using the phonon model.
- 2. To derive the frequency spectrum of the black body radiation.
- 3. To derive the condensation temperature of a Bose-Einstein condensate.

**Statistical and Low Temperature Physics
(PHYS393)**

6. Photons and phonons

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We can count the number of states for the phonons, like we did for atoms in an ideal gas, or electrons in a metal.

Unlike electrons, however, the exclusion principle does not apply to phonons.

So each energy state can be occupied by any number of phonons.

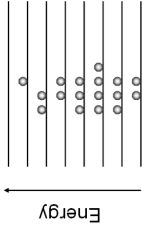
This means that we need yet another way to find the macrostate. This was worked out by Bose and Einstein in the 1920s.

Bose-Einstein Statistics

The method is similar to what we have used for the ideal gas.

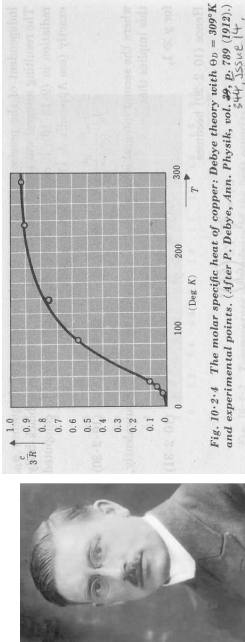
There, we have made the assumption that there are many more energy levels than there are particles. This has meant that it is unlikely for two gas atoms to occupy the same state.

We do not make this assumption now, since we would be particularly interested in the low temperature behaviour.



Since the exclusion principle does not apply to phonons, more than one phonons can occupy the same state.

Previously, we have looked at Einstein's model of the 3-D simple harmonic oscillator, in which each atom in a solid is in its own potential well. The predicted heat capacity was accurate at high temperature, but fails at low temperature.

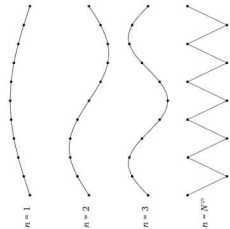


In 1912, Peter Debye, a Dutch physicist working in Germany, produced a theory which turns out to be very accurate both hot and cold.

Atoms vibrating in a solid

In Debye's model, we think of the atoms in a solid as connected by springs. They vibrate in 3D in a complicated way.

The problem can be simplified by treating the vibration as a superposition of waves of different frequencies.



If we suppose that the atoms are fixed at the edge of the solid, the frequency would be quantised. A quantum of this vibration energy is called a phonon.

Phonons are not real particles like atoms or electrons. The number of phonons is related to the vibration energy. The number would increase when the temperature increases. At 0 Kelvin, there is no vibration, so there would be no phonons.

Because of this, there would be no constraint on the number N . We really only have one constraint - that of constant energy U .

The Lagrange function is $\ln \Omega + \lambda U$. N does not appear. Maximising this function, we get

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda \varepsilon_i) - 1}.$$

With the help of entropy as before, we would find

$$\lambda = -\frac{1}{k_B T}.$$

Phonon occupation number

Maximising Lagrange function, we have obtained

$$\frac{n_i}{g_i} = \frac{1}{\exp(\varepsilon_i/k_B T) - 1}.$$

Following the same notations that we have used for ideal gas and electrons, we rewrite:

$$n_i \text{ as } n(\varepsilon)d\varepsilon \text{ and} \\ g_i \text{ as } g(\varepsilon)d\varepsilon.$$

This gives

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

Next, we need a formula for the density of states $g(\varepsilon)$.

Note that although we have previously used the same symbol $g(\varepsilon)$ for the particle in a 3-D box, the phonon density of states would have a different formula.

Suppose, in the energy bundle i , that there are g_i levels and n_i phonons. The phonons are now completely free to arrange themselves among the energy levels.

This means that we have $n_i + g_i$ objects altogether in the bundle. There are n_i of one type, and g_i of the other type. The number of possible arrangements would be

$$\Omega_i = \frac{(n_i + g_i)!}{n_i! g_i!}$$

The total number of arrangements for all bundles would be obtained by multiplication of the number for every bundle:

$$\Omega = \prod_i \frac{(n_i + g_i)!}{n_i! g_i!}.$$

Bose-Einstein Distribution

Then we need to maximise $\ln \Omega$ using the Lagrange multiplier method.

Using the same constraints as before on the number of particles N and the total energy U , the method would give the following answer:

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda_1 - \lambda_2 \varepsilon_i) - 1}.$$

where λ_1 and λ_2 are the Lagrange multipliers.

This is called the Bose-Einstein distribution function. It looks almost the same as the Fermi-Dirac distribution function, except that it has -1 in the denominator instead of +1.

When we apply this to phonon, however, we need to make some changes.

Defining k as the magnitude of the wave vector, we have

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

and

$$k^2 = \frac{\omega^2}{v^2}.$$

The boundary condition requires ξ to be zero at the walls. Therefore, in the same way as the particle in the box, the wavevector would be quantised:

$$k_x = \frac{n_x \pi}{a}, \quad k_y = \frac{n_y \pi}{a} \quad \text{and} \quad k_z = \frac{n_z \pi}{a}.$$

Substituting these into

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

gives

$$k^2 = \frac{\pi^2}{a^2}(n_x^2 + n_y^2 + n_z^2)$$

Rearranging,

$$\frac{k^2 a^2}{\pi^2} = n_x^2 + n_y^2 + n_z^2.$$

We have also obtained above the dispersion relation

$$k = \frac{\omega}{v}.$$

Substituting,

$$\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2 + n_y^2 + n_z^2.$$

We may now follow the same method that we have used for ideal gas to count the states. Comparing with the equation for a sphere

$$R^2 = n_x^2 + n_y^2 + n_z^2$$

the total number of states with frequency less than ω is given by the octant of the sphere:

$$G(\omega) = \frac{1}{8} \left(\frac{4\pi}{3} R^3 \right) = \frac{\pi}{6} \left(\frac{\omega a}{v\pi} \right)^3$$

The vibrations in a solid is described by the wave equation

$$\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 \xi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \xi}{\partial t^2}$$

where ξ is related to the displacement of the atoms.

http://en.wikipedia.org/wiki/Wave_equation

The solution has a similar form to the wave function for the particle in a box:

$$\xi = e^{i\omega t} \sin k_x x \sin k_y y \sin k_z z$$

where ω is the angular frequency.

Substituting the solution for ξ into the wave equation above, we would get

$$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{v^2}.$$

Substituting into the wave equation would be easier if we work out each of the partial derivatives first. For example, differentiating twice with respect to x , we would get

$$\frac{\partial^2 \xi}{\partial x^2} = e^{i\omega t} (-k_x^2 \sin k_x x) \sin k_y y \sin k_z z = -k_x^2 \xi.$$

Likewise with respect to y and z . Differentiating twice with respect to t , we would get

$$\frac{\partial^2 \xi}{\partial t^2} = (-\omega^2 e^{i\omega t}) \sin k_x x \sin k_y y \sin k_z z = -\omega^2 \xi.$$

Now we can see that substituting into the wave equation gives

$$-k_x^2 \xi - k_y^2 \xi - k_z^2 \xi = \frac{1}{v^2} (-\omega^2 \xi),$$

which is

$$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{v^2}.$$

There is one more practical point to note. In a solid, there is a limit to the highest phonon frequency.

This is related to the fact that the wavelength cannot possibly be shorter than the distance between atoms.

Let this highest frequency be ω_D .

In a solid with N identical atoms, there are $3N$ energy states, or normal modes. This is when we count every possible frequency, and every possible "direction of vibration" for each frequency.

This can be proven mathematically, but we shall skip that. We can find ω_D by integrating the density of states:

$$\int_0^{\omega_D} g(\omega) d\omega = \int_0^{\omega_D} \frac{3V\omega^2 d\omega}{2\pi^2 v^3} = 3N$$

This equation

$$\int_0^{\omega_D} g(\omega) d\omega = \int_0^{\omega_D} \frac{3V\omega^2 d\omega}{2\pi^2 v^3} = 3N$$

can then be solved to find the Debye frequency. Integrating gives

$$\frac{V\omega_D^3}{2\pi^2 v^3} = 3N$$

Solving for ω_D gives the Debye frequency:

$$\omega_D = \left(\frac{6N\pi^2 v^3}{V} \right)^{1/3}$$

Differentiating the number of states,

$$G(\omega) = \frac{\pi}{6} \left(\frac{\omega a}{v\pi} \right)^3$$

we get the density of states:

$$g(\omega) = \frac{V\omega^2}{2\pi^2 v^3}$$

where V is the volume a^3 .

Actually, we are not quite there yet.

There reason is that each state correspond to a wave, and a wave in a solid can have 2 transverse polarisations, and 1 longitudinal polarisation.

Previously, we have only counted the states in terms of the possible wavevector (n_x, n_y, n_z) . In the case of solids, the 3 different directions of vibrations are in fact different states with the same wavevector (n_x, n_y, n_z) .

So we have to multiply by 3 to get the correct density of state:

$$g(\omega) d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

The phonon distribution is given by

$$n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

We can multiply by $\hbar\omega$ to get the energy at this frequency interval:

$$\hbar\omega n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

The total energy is then

$$U = \int_0^{\omega_D} \hbar\omega n(\omega)d\omega = \int_0^{\omega_D} \frac{\hbar\omega g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

We have found earlier that the density of states is:

$$g(\omega) = 3 \times \frac{V\omega^2}{2\pi^2 v^3}.$$

Substituting into the integral for the total energy above ...

Debye's theory for Heat capacity of solid

We get:

$$U = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3 d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

At low temperature, it can be shown that this is proportional to T^4 . This would imply that the heat capacity C is proportional to T^3 . (This has been mentioned in the topic on the specific heat of electrons in metal.)

At high temperatures, the heat capacity tends to $3Nk_B$.

As we have shown earlier, the distribution of phonons is given by

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

We shall express this in terms of frequency ω as well. The phonon energy ε is given by

$$\varepsilon = \hbar\omega.$$

This is a result of the phonon mode

$$\xi = e^{i\omega t} \sin k_x x \sin k_y y \sin k_z z$$

behaving as a simple harmonic oscillator. The phonon mode is simply vibration of the atoms co-ordinated in a particular way.

The phonon distribution

So the energy must take the form

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega.$$

Each step or quantum is $\hbar\omega$, which would be interpreted as a phonon particle in our statistical treatment. The relation

$$\varepsilon = \hbar\omega$$

would be justified by the fact that its predictions agree with experiments.

In terms of the frequency ω , the phonon distribution is then given by

$$n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

If you are using the recommended text:

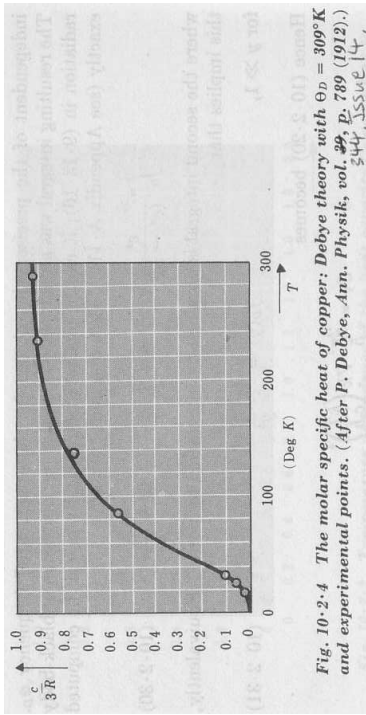
Statistical Mechanics - A Survival Guide,
by A. M. Glazer and J. S. Wark

please note that the Lagrange multiplier method given on page
72 is incorrect.

Please use the version given in these lectures.

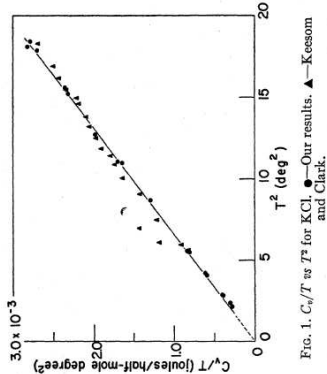
6.2 Photons

In 1912, Debye measured the high temperature behaviour of copper.



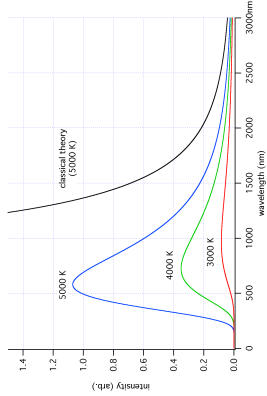
He showed that the heat capacity did tend to $3Nk_B$, as he had predicted.

In 1953, at Purdue University, Keesom and Pearlman measured the low temperature behaviour of potassium chloride.



P. H. Keesom and N. Pearlman, *Physical Review*, vol. 91 (1953), pp. 1354-1355

As predicted by Debye, the heat capacity was indeed proportional to T^3 .



http://en.wikipedia.org/wiki/Black_body

As the temperature decreases, the peak of the black-body radiation curve moves to lower intensities and longer wavelengths. The black-body radiation graph is also compared with the classical model of Rayleigh and Jeans.

Photons in a box

We can derive a formula for the black body radiation by considering the energies of photons in a box (like a idea black body).

This follows steps very similar to the Debye theory for phonons.

The wave equation for photons is derived from Maxwell's equation:

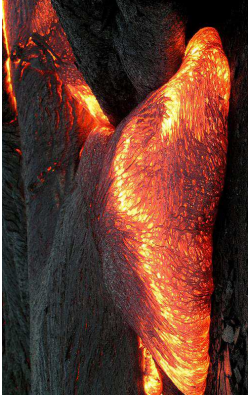
$$\frac{\partial^2 \mathbf{E}}{\partial x^2} + \frac{\partial^2 \mathbf{E}}{\partial y^2} + \frac{\partial^2 \mathbf{E}}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

It has the same form as the wave equation for vibration of atoms, except that the speed is now that of light instead of sound.

So we would expect that the same formula for the density of states can be used.

When an object gets very hot, it can give out light.

The temperature of a volcano lava flow can be estimated by observing its color. The result agrees well with the measured temperatures of lava flows at about 1,000 to 1,200 deg C.



http://en.wikipedia.org/wiki/Black_body

An ideal black body

The amount of radiation emitted depends on the nature of the object - its colour, whether it is smooth or rough, etc.

An ideal black body is one that absorbs all the radiation that falls on it.

No real material can do this. Soot is about the best, absorbing all but 3%.

In 1859 Kirchhoff had a good idea: "a small hole in the side of a large box is an excellent absorber, since any radiation that goes through the hole bounces around inside, a lot getting absorbed on each bounce, and has little chance of ever getting out again."

http://galileo.phys.virginia.edu/classes/252/black_body_radiation.html

The energy of the absorbed radiation reaches equilibrium among different frequencies in the cavity. This results in a characteristic spectrum that would be emitted again through the hole.

| Photons in a box | Distribution of photon number |
|--|---|
| <p>Like phonons, the photon number is not fixed. We get few photons when the box is cold, and more photons when it is hot.</p> <p>Unlike phonons, there is no upper limit to the frequency (no Debye frequency). The wavelength in a solid cannot be shorter than the distance between atoms. The electromagnetic wave in a box has no such limit.</p> <p>Finally, phonons in a solid can have 3 polarisations: 2 transverse and 1 longitudinal (like sound). Photons can only have 2: both transverse (e.g. light).</p> | <p>Like phonons, each energy state can be occupied by any number of photons.</p> <p>So it obeys Bose-Einstein statistics.</p> <p>The number density is therefore given by the same formula:</p> $n(\epsilon)d\epsilon = \frac{g(\epsilon)d\epsilon}{\exp(\epsilon/k_B T) - 1}$ <p>So the number of photons in a given frequency interval is</p> $n(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 c^3} \times \frac{d\omega}{\exp(\hbar\omega/k_B T) - 1}$ |
| PHYS393/Hock | PHYS393/Hock |
| 32 | 34 |
| 2009-2010 | 2009-2010 |
| Counting photon states | Distribution of photon energy |
| <p>Recall that for phonons, the density of states is give by:</p> $g(\omega)d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$ <p>where the factor of 3 comes from the 3 polarisations of a phonon, 2 transverse and 1 longitudinal.</p> <p>Since photons only have 2 polarisations, both transverse, the 3 should be replaced by a 2:</p> $g(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 c^3}$ <p>where the sound speed v is replaced by light speed c.</p> | <p>The energy of a photon is $\hbar\omega$. The energy in the frequency interval $d\omega$ is then</p> $\hbar\omega n(\omega)d\omega = 2 \times \hbar\omega \times \frac{V\omega^2 d\omega}{2\pi^2 c^3} \times \frac{d\omega}{\exp(\hbar\omega/k_B T) - 1}$ <p>The energy density is given by:</p> $u(\omega) = \hbar\omega n(\omega) = \frac{V\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}.$ <p>This is essentially Planck's law for black body radiation. Integrating gives the total energy:</p> $U = \frac{\pi^2 V k_B^4}{15 \hbar^3 c^3} T^4$ <p>It can be shown that this leads to Stefan's law of radiation:</p> $\eta = \sigma T^4$ <p>for radiation emitted by an object at a temperature T.</p> |
| PHYS393/Hock | PHYS393/Hock |
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| 2009-2010 | 2009-2010 |

Berlin, 1899. In the Imperial Institute of Physics and Technology, the scientists were just trying to help the German lighting and heating industries.



**Otto
Lummer
1860-1925**

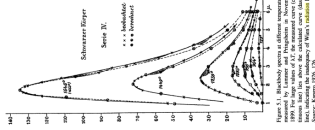


**Ernst
Pringsheim
1859-1917**

Lummer and Pringsheim measured the radiation spectrum from a blackbody very accurately.

Blackbody radiation

The results did not look at all like what the physicists thought it should.



**Lummer-type
photometer**

Then Max Planck came along and derived his formula for black body radiation that agreed very well with these measurements. And the rest is history.

6.3 Bose-Einstein Condensation

Bosons

We have seen that for phonons and photons, any number of such particles can occupy the same energy state.

Such particles are called bosons. They have integer spin.

E.g. phonon has spin 0, and photon has spin 1.

Atoms can also have integer spin number.

For example, (¹⁴O) oxygen-14 atom and the (⁴He) helium-4 atom are bosons.

Cornell and Wieman observed the BEC for the first time.

At first, they saw the expected distribution of velocities (left) in a gas. Then the graph becomes a single peak (right). This means that all atoms have achieved the same velocity - i.e. become a BEC.

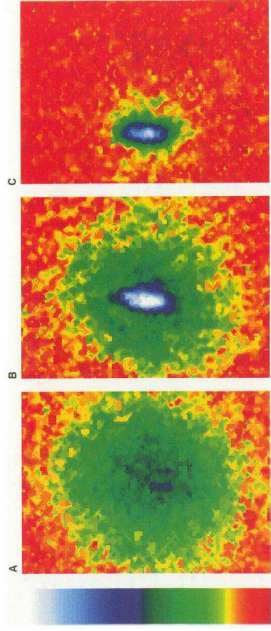


Fig. 2. False-color images display the velocity distribution of the cloud (A) just before the appearance of the condensate, (B) just after the appearance of the condensate, and (C) after formation of the condensate fraction (mostly blue and green) is an indication that the velocity distribution is isotropic, consistent with thermal equilibrium. The condensate fraction (mostly blue and white) is elliptical, indicative that it is a highly nonthermal distribution. The elliptical pattern is the result of the anisotropy of the magnetic field used to trap the condensate. The field of view of each image is 200 μm by 270 μm . The observed horizontal width of the condensate is broadened by the experimental resolution.

When do the bosons condense?

Using the Bose-Einstein distribution that we have learnt, we can calculate the temperature at which bosons condense into BEC.

Recall the expression we first derived for the Bose-Einstein distribution:

$$\frac{n_i}{g_i} = \frac{1}{\exp(-\lambda_1 - \lambda_2 \epsilon_i) - 1}$$

When applying this to phonons, λ_1 was left out because the number of phonons is not fixed.

Now that we are dealing with atoms, which are real bosons, the number is fixed and we have to keep λ_1 . This is usually written in terms of μ as follows:

$$n(\epsilon)d\epsilon = \frac{g(\epsilon)d\epsilon}{\exp((\epsilon - \mu)/k_B T) - 1}$$

Phonons and photons can appear or disappear when an object is heated or cooled. They are called virtual bosons.

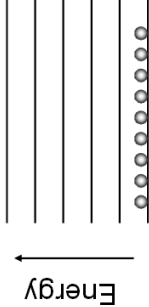
Atoms, however, cannot just appear or disappear. Those with integer spin number are called real bosons.

Like phonons and photons, any number of such bosonic atoms can occupy the same energy state.

This gives rise to a curious state of matter called Bose-Einstein Condensate.

What is Bose Einstein Condensate (BEC)?

When it gets cold enough all boson particles can fall into the ground state.



These particles then behave as if they are a single particle with a single wavefunction - all of them with the same velocity!

We focus on the occupation number in the integral:

$$f(\varepsilon) = \frac{1}{\exp((\varepsilon - \mu)/k_B T) - 1}$$

First, note that μ cannot be positive, or else for small energy the exponential function would be less than one. Then the denominator would be negative. This means negative occupation number, which is not physical.

Next, we know that when temperature is low enough, a large number of atoms would go into the ground state $\varepsilon = 0$. The number would be as large as N , which is of the order of 1 mole ($\approx 10^{24}$).

This means that $f(0)$ would be very large, so that μ must be very close to zero. Then the exponential function would be close to 1 and the denominator would be close to zero.

Number of atoms in the excited state

So at very low temperature, it is safe to assume that $\mu = 0$. We can then write

$$N_{ex} = \int_0^\infty \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

I have added a subscript *ex* to N . The reason will become clear in a moment. First, integrate this with the help of the Table of Integrals:

$$N_{ex} = \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} 2.612V$$

Notice that T is in the denominator. This suggests that the total number of atoms decreases with temperature - that they are disappearing !

In fact, the above integral includes only atoms above the ground state $\varepsilon = 0$. The "missing" atoms are in fact going into the ground state.

We have seen a number of different density of states.

For electrons, we need to multiply by 2 because of the spin states. For phonons, we multiply by 3 for the three possible polarisationz. For photons, we multiply by 2 for the two polarisation states.

So what do we do for atoms that are bosons?

The answer is: we use the same density of state for the ideal gas:

$$g(\varepsilon) = \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2}$$

This is the very first one that we have seen, before we have to include the additional effects of spin and polarisation.

The chemical potential

μ is called the chemical potential. It is determined by the total number of particles. We get this by integrating:

$$N = \int_0^\infty \frac{g(\varepsilon)d\varepsilon}{\exp((\varepsilon - \mu)/k_B T) - 1}$$

I have assumed that the ground state energy is zero, which is why I integrated from zero.

This is not easy to solve. Instead, we shall make use of some approximations at low temperature.

For a start, note that μ could depend on temperature, since the above equation contains T .

When Cornell and Wiemann observed the first BEC in Colorado, they used rubidium gas with a condensation temperature of 1.7×10^{-7} K.

This is far below the temperature that can be reached using liquid helium (melting point 4.2 K).

They have to use a special method called laser cooling.

For more information on laser cooling, see:

http:
http://physweb.bgu.ac.il/COURSES/LAB_C/Laser%20Cooling%20and%20trapping/colorado%20mot.pdf
http://en.wikipedia.org/wiki/Laser_cooling

What we have learnt so far.

1. The Bose-Einstein distribution function is given by

$$f(\epsilon) = \frac{1}{\exp[(\epsilon - \mu)/k_B T] - 1}.$$

2. For phonons and photons, the following form is used:

$$f(\epsilon) = \frac{1}{\exp(\epsilon/k_B T) - 1}.$$

3. The density of states can take different forms:

phonons

$$g(\omega)d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

photons

$$g(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

bosonic atoms

$$g(\epsilon) = \frac{4m\pi V}{h^3}(2m\epsilon)^{1/2}$$

The formula for N_{ex} is only able to compute the number of particles above the ground state. This is because the density of states $g(\epsilon)$ in the integral is zero when $\epsilon = 0$.

When a substantial fraction of the particles start going into the ground state, this has to be added separately. So N_{ex} is the number of atoms in the excited states. Hence the subscript *ex*.

We know that as soon as N_{ex} becomes less than the original number N , then $(N - N_{ex})$ atoms start going into the ground state.

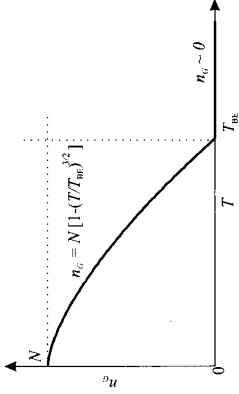
Therefore, condensation takes place when $N_{ex} = N$. Substituting this and solving for T , we get

$$T_{BE} = \frac{h^2}{2\pi m k_B} \left(\frac{N}{2.612V} \right)^{2/3}.$$

Number of atoms in the ground state

Above T_{BE} , there are very little atoms in the ground state.

Below T_{BE} , this number increases until all atoms fall into the ground state.



Glazer and Wark, Statistical mechanics, p. 101

Exercise 1

Sketch the density of states as a function of frequency for 1, 2 and 3-D solids in the Debye approximation. Consider a 2-D solid. Show according to the Debye theory that the heat capacity varies as T^2 at low temperature. In graphite it is found that $C_V \propto T^{2.4}$ at low temperature. Explain this behaviour.

Exercises

Recall the steps leading to the density of states of a phonon in a 3-D solid. First, we obtain the quantised energy states:

$$\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2 + n_y^2 + n_z^2.$$

Then we compare with the equation for a sphere

$$R^2 = n_x^2 + n_y^2 + n_z^2$$

For positive integers (n_x, n_y, n_z) , the total number of states with frequency less than ω is given by the octant of the sphere:

$$G(\omega) = \frac{1}{8} \left(\frac{4\pi}{3} R^3 \right) = \frac{\pi}{6} \left(\frac{\omega a}{v\pi} \right)^3$$

Differentiating, we get the density of states:

$$g(\omega) = 3 \times \frac{V\omega^2}{2\pi^2 v^3}$$

where V is the volume a^3 . There is an extra factor of 3 because in 3-D, there can be 3 modes for each phonon frequency: 2 transverse and 1 longitudinal.

electrons

$$g(\varepsilon) = 2 \times \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2}$$

classical ideal gas

$$g(\varepsilon) = \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2}$$

3. At low temperature, the specific heat capacity for the Debye model tends to T^3 . At high temperature, it tends to $3Nk_B$.

4. The energy distribution in a photon gas is given by:

$$u(\omega) = \hbar\omega n(\omega) = \frac{V\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}.$$

This also describes the black body radiation spectrum.

7. The condensation temperature for a Bose-Einstein condensate is:

$$T_{BE} = \frac{h^2}{2\pi m k_B} \left(\frac{N}{2.612V} \right)^{2/3}.$$

6.4 Exercises

| density of states for phonons | |
|--|--|
| Now we repeat the steps for 2-D. First, we obtain the quantised energy states (no n_z): | |
| | $\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2 + n_y^2.$ |
| Then we compare with the equation for a circle (not sphere) | $R^2 = n_x^2 + n_y^2$ |
| For positive integers (n_x, n_y), the total number of states with frequency less than ω is given by the quadrant of the circle (not octant): | $G(\omega) = \frac{1}{4}(\pi R^2) = \frac{\pi}{4} \left(\frac{\omega a}{v \pi} \right)^2$ |
| Differentiating, we get the density of states: | $g(\omega) = 2 \times \frac{A \omega}{2 \pi v^2}$ |
| where A is the area a^2 (not volume). There is an extra factor of 2 because in 2-D, there can be 2 modes for each phonon frequency: 1 transverse and 1 longitudinal. | |
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| Exercises | |
|--|--|
| Summarising, we have obtained the following results for the density of states: | |
| 1-D: $g(\omega) = \text{constant}$ | |
| 2-D: $g(\omega) \propto \omega$ | |
| 3-D: $g(\omega) \propto \omega^2$ | |
| The internal energy is given by: | $U = \int_0^{\omega_D} \frac{\hbar \omega g(\omega) d\omega}{\exp(\hbar \omega / k_B T) - 1}.$ |
| In 2-D, | |
| So | $U \propto \int_0^{\omega_D} \frac{\omega^2 d\omega}{\exp(\hbar \omega / k_B T) - 1}.$ |
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| Exercises | |
|--|--|
| Finally we repeat the steps for 1-D. First, we obtain the quantised energy states (no n_y): | $\frac{\omega^2 a^2}{v^2 \pi^2} = n_x^2.$ |
| Then we compare with the equation for a line (not circle) | $R^2 = n_x^2$ |
| For positive integers n_x , the total number of states with frequency less than ω is given by half of the line (not quadrant): | $G(\omega) = \frac{1}{2}(2R) = \frac{\omega a}{v \pi}$ |
| Differentiating, we get the density of states: | $g(\omega) = 1 \times \frac{L}{\pi v}$ |
| where L is the length a (not area). There is no additional factor because in 1-D, there can be only be 1 mode for each phonon frequency: the longitudinal. | |
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| Exercises | |
|---|--|
| We have obtained | $U \propto \int_0^{\omega_D} \frac{\omega^2 d\omega}{\exp(\hbar \omega / k_B T) - 1}.$ |
| Let | $x = \frac{\hbar \omega}{k_B T}.$ |
| At low temperature, $T \rightarrow 0$ and $x \rightarrow \infty$. The integral for U can be written as | $U \propto T^3 \int_0^{\infty} \frac{x^2 dx}{e^x - 1}.$ |
| The factor of T^3 appears because of the factor of T in the substitution for ω : | $\omega = \frac{k_B T}{\hbar} x.$ |
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To use the formula given, let the argument of the exponential function be x :

$$x = \frac{\hbar\omega}{k_B T}.$$

Make frequency the subject:

$$\omega = \frac{k_B T}{\hbar} x.$$

Then substitute into the integral for the energy:

$$U = \frac{3V\hbar}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar} \right)^4 \int_0^{x_D} \frac{x^3 dx}{e^x - 1}$$

where the new limit is related to the old one by the substitution formula:

$$x_D = \frac{\hbar\omega_D}{k_B T}.$$

The condition given is $T \ll \hbar\omega_D/k_B$. Rearranging, we have

$$1 \ll \frac{\hbar\omega_D}{k_B T}.$$

The right hand side is just x_D , so

$$1 \ll x_D.$$

This means x_D is large. We may approximate the integral by replacing the limit by infinity:

$$U \approx \frac{3V\hbar}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar} \right)^4 \int_0^\infty \frac{x^3 dx}{e^x - 1}.$$

Then using the formula given,

$$U = \frac{3V\hbar}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar} \right)^4 \frac{\pi^4}{15}.$$

Since the definite integral here

$$U \propto T^3 \int_0^\infty \frac{x^2 dx}{e^x - 1}.$$

is a constant, we have

$$U \propto T^3.$$

Differentiating, the heat capacity is

$$C_V \propto T^2.$$

Graphite has a layered structure. Each layer consists of carbon atoms strongly bonded, with weak forces between layers. Vibration (like sound) would propagate much faster along the layer than across the layers. So it can be thought of as intermediate between 2-D and 3-D.

This explains why the heat capacity of graphite is

$$C_V \propto T^{2.4}.$$

Exercise 2

According to Debye's theory, the total energy of phonons in a solid is given by

$$U = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3 d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

Show that at low temperatures, i.e. $T \ll \hbar\omega_D/k_B$, Debye's theory predicts that the heat capacity of a solid is proportional to T^3 .

[You are given that

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}.$$

]

Recall that x_D is related to the Debye frequency by

$$x_D = \frac{\hbar\omega_D}{k_B T},$$

This means that for 1% accuracy, we should have

$$\frac{\hbar\omega_D}{k_B T} > 10.$$

Rearranging, we get

$$T < \frac{\theta_D}{10}$$

where

$$\theta_D = \frac{\hbar\omega_D}{k_B}.$$

θ_D is called the Debye temperature, and can be used as a reference when we want to tell whether a temperature is high or low. Note that in the numerator is $\hbar\omega_D$, which is the highest possible phonon energy.

Exercise 3

The energy distribution of a gas of photons in a box given by:

$$u(\omega)d\omega = \frac{V\hbar}{\pi^2 c^3} \frac{d\omega}{\omega^3} \frac{\exp(\hbar\omega/k_B T) - 1}{\omega^3}.$$

Wien's displacement law for black body radiation is given by

$$\lambda_{\max} = \frac{b}{T},$$

where λ_{\max} is the wavelength of the peak of the radiation intensity, and b is 2.90×10^{-3} m.K.

Derive Wien's displacement law from the energy distribution.

We have found the total energy.

$$U = \frac{V\pi^2 k_B^4 T^4}{10\hbar^3 v^3}$$

Note that this is proportional to T^4 . To get the heat capacity, we differentiate with respect to temperature T :

$$C = \frac{2V\pi^2 k_B^4 T^3}{5\hbar^3 v^3}$$

which is proportional to T^3 .

This answers the question.

Some remarks:

Going back to our approximation, how large must x_D be for the approximation

$$\int_0^{x_D} \frac{x^3 dx}{e^x - 1} \approx \int_0^\infty \frac{x^3 dx}{e^x - 1}$$

to be valid? We can get some idea if we carry out the integration numerically:

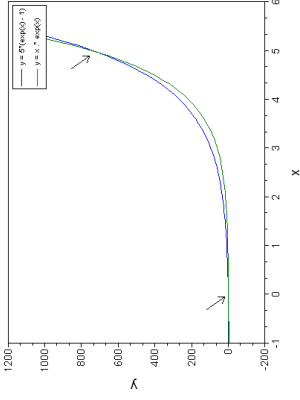
| x_D | $\int \frac{x^3 dx}{e^x - 1}$ | error |
|----------|-------------------------------|------------|
| 1 | 0.225 | 96% |
| 10 | 6.432 | 1% |
| 100 | 6.494 | 10^{-18} |
| ∞ | $\pi^4/15$ | 0 |

As long as x_D is more than 10, the approximation would be better than 1%.

If we plot each side of the equation,

$$5(e^x - 1) = xe^x.$$

we see that there are 2 solutions.



We can solve this numerically. The answers are

$$x_1 = 0 \quad \text{and} \quad x_2 = 4.965.$$

Exercises

The nontrivial solution is

$$x_2 = 4.965.$$

Substituting this into the definition for x ,

$$x = \frac{h}{\lambda k_B T}.$$

or making λ the subject, we get

$$\lambda = \frac{hc}{x_2 k_B T}.$$

Comparing this with the displacement law,

$$\lambda_{\max} = \frac{b}{T},$$

we see that

$$b = \frac{hc}{x_2 k_B}.$$

Substituting the constants and calculating, we get the Wien's displacement constant 2.90×10^{-3} m.K.

Exercises

We must rewrite the distribution in terms of wavelength λ :

$$\omega = 2\pi f = 2\pi \frac{c}{\lambda}$$

Differentiating,

$$d\omega = -\frac{2\pi c}{\lambda^2} d\lambda.$$

Substituting into the energy distribution:

$$u(\lambda)d\lambda = \frac{Vh}{\pi^2 c^2 \lambda^5} \frac{d\lambda}{\exp(hc/\lambda k_B T) - 1}.$$

To find the maximum, we can ignore the constants in $u(\omega)$ and just focus on the part that depends on ω :

$$\frac{1}{\lambda^5} \frac{1}{\exp(hc/\lambda k_B T) - 1}.$$

To find the maximum, differentiate this ...

Exercises

and set to zero:

$$-\frac{5}{\lambda^6} \frac{1}{\exp(hc/\lambda k_B T) - 1} - \frac{1}{\lambda^5} \frac{(-hc/\lambda^2 k_B T) \exp(hc/\lambda k_B T)}{[\exp(hc/\lambda k_B T) - 1]^2} = 0.$$

Multiplying by $\lambda^6 [\exp(hc/\lambda k_B T) - 1]^2$,

$$-5[\exp(hc/\lambda k_B T) - 1] + \frac{hc}{\lambda k_B T} \exp(hc/\lambda k_B T) = 0.$$

We can simplify this by defining

$$x = \frac{hc}{\lambda k_B T}.$$

Substituting, we get

$$-5(e^x - 1) + xe^x = 0.$$

Exercise 5

Show that below the condensation temperature, T_{BE} , the heat capacity of a gas obeying Bose-Einstein statistics is given by

$$C_V = 1.93 N k_B \left(\frac{T}{T_{BE}} \right)^{3/2}.$$

[You are given that

$$\int_0^\infty \frac{x^{3/2}}{e^x - 1} dx = 1.78.$$

]

Exercises

Recall that at very low temperatures, the chemical potential μ is approximately zero, and the number of particles above the ground state is given by:

$$N_{ex} = \int_0^\infty \frac{g(\varepsilon) d\varepsilon}{\exp(\varepsilon/k_B T) - 1}.$$

To obtain the energy, we insert ε into the integral:

$$U = \int_0^\infty \frac{g(\varepsilon) \varepsilon d\varepsilon}{\exp(\varepsilon/k_B T) - 1}.$$

Substituting the density of states

$$g(\varepsilon) = \frac{4m\pi V}{h^3} (2m\varepsilon)^{1/2}$$

gives

$$U = \frac{4m\pi V}{h^3} \int_0^\infty \frac{\sqrt{2m\varepsilon}^{3/2} d\varepsilon}{\exp(\varepsilon/k_B T) - 1}.$$

Exercise 4

Bose-Einstein condensation is achieved with a gas of rubidium atoms, which have an atomic weight of 85.47. The condensation temperature is 1.7×10^{-7} K. What was the number density of the condensate?

[Atomic mass unit u is 1.6605×10^{-27} kg.]

Exercises

Recall the formula for the condensation temperature:

$$T_{BE} = \frac{h^2}{2\pi m k_B} \left(\frac{N}{V} \right)^{3/2}$$

We can rearrange this to get the number density:

$$\frac{N}{V} = 2.612 \left(\frac{2\pi m k_B T_{BE}}{h^2} \right)^{3/2}$$

The condensation temperature is given as

$$T_{BE} = 1.7 \times 10^{-7} \text{ K}.$$

The mass is given by

$$m = 85.47 u = 85.47 \times (1.6605 \times 10^{-27}) \text{ kg}.$$

Substituting these into the above equation for the number density, we get $2.74 \times 10^{19} \text{ m}^{-3}$.

Define

$$x = \frac{\varepsilon}{k_B T}$$

and substitute into the integral for energy:

$$U = \frac{4m\pi V}{h^3} \sqrt{2m}(k_B T)^{5/2} \int_0^\infty \frac{x^{3/2} dx}{e^x - 1}.$$

We can now use the given result:

$$\int_0^\infty \frac{x^{3/2}}{e^x - 1} dx = 1.78.$$

This gives:

$$U = \frac{4m\pi V}{h^3} \sqrt{2m}(k_B T)^{5/2} \times 1.78.$$

The heat capacity can then be obtained by differentiating this with respect to temperature. First, we express this in terms of the condensation temperature.

Exercises

The condensation temperature is given by:

$$T_{BE} = \frac{h^2}{2\pi m k_B} \left(\frac{N}{2.612V} \right)^{3/2}$$

Make V the subject

$$V = \frac{1}{2.61} \left(\frac{h^2}{2\pi m k_B T_{BE}} \right)^{3/2}$$

and substitute into the above result for U :

$$U = \frac{2}{\sqrt{\pi}} \frac{1.78}{2.61} N k_B \frac{T^{5/2}}{T_{BE}^{5/2}}$$

Then differentiating with respect to T :

$$C_V = 1.93 N k_B \left(\frac{T}{T_{BE}} \right)^{3/2}$$

we get the heat capacity for the Bose-Einstein condensate.